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Inverse Problem in Explosion and Combustion

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The principal task of our studies is to provide a rational interpretation of the thermodynamic and fluid dynamic events taking place in a closed vessel upon detonation of an explosive charge and subsequent turbulent combustion of its products, acting as fuel for an exothermic reaction with air. Under such circumstances, the latter has been compressed by a reverberating shock front of the blast wave generated by the explosion. The paper presents the chemical and thermodynamic background and its numerical results, deduced for this purpose from mass spectroscopic data and pressure records, acquired upon explosion of a 0.8 kg charge of TNT in a 17 m³ chamber filled with air – a diagnostic analysis identified by the title. The evolution of the flow field and its structure are presented in a companion paper¹.

Chemical background

Considered here, in particular, are tests for which the charge was made out of 875 gm of TNT, contained in an enclosure 16.6 m³ in volume, filled with 20 kg of either nitrogen or air at 1 bar and 300K. The chemical composition of fuel for the post-explosion combustion was determined from mass spectroscopic measurement of “post-shot” products of TNT explosion in nitrogen. The data were incomplete, in that they did not include the concentrations of C, H₂O and N₂. Their fractions were deduced from stoichiometric analysis of the chemical reaction, taking place in the course of explosion, namely



or, in terms of the measured mole fractions, X_{oi} ,



Atom balances of (2) yield four equations:

$$O: [2X_{o1} + X_{o2} + 2X_{o5}] \alpha + v_8 = 6 \quad (3)$$

$$H: [4X_{o3} + 2X_{o4}] \alpha + 2v_8 = 5 \quad (4)$$

$$C: [X_{o1} + X_{o2} + X_{o3}] \alpha + v_7 = 7 \quad (5)$$

$$N: 2v_6 = 3 + 2v_n \quad (6)$$

yielding the values of α , together with those of v_6 , v_7 and v_8 , whence $v_i = \alpha X_{oi}$ for $i = 1-4$, and, concomitantly, $X_i = v_i / \Sigma v_i$.

Thermodynamic background²

An exothermic process of combustion is carried out in three steps:

1. initiation (by ignition or compression), governed by molecular diffusion, devoid of a productive pressure yield
2. dynamic stage, manifested by a monotonic pressure rise, furnishing the potential for work
3. decay, dominated by molecular and thermal diffusion at the walls, associated with energy loss due to heat transfer, terminating the productive pressure rise.

Of primary relevance to the dynamic features of combustion is, of course, the second stage, forming, therefore, the main subject of our studies. At its kernel is a chemical reaction, whereby a mixture, M, of fuel, F, and air, A, is converted into products, P, whose composition is specified by its thermodynamic equilibrium. Depending on the purpose of the analysis, $M = S, R$, the first referring to the whole system, and the second to the stoichiometric mixture of A with F. Salient features of the thermodynamic proper-

¹ Kuhl, A.L., Oppenheim, A.K., & Ferguson, R.E., 18th ICDERS, 2001

² Presented here is an updated and abridged version of our previous publications on the thermodynamic method of approach to the analysis of closed combustion systems, in particular: [1] Oppenheim, A.K. & Kuhl, A.L., *Archivum Combustionis*, vol. 19, no. 1-4, pp. 15-65, 1999; [2] Oppenheim, A.K. & Kuhl, A.L., *Progress in Energy and Combustion Science*, vol. 26, pp. 533-564, 2000

ties of fuel, F, and air, A, as well as of their mixture, M, and the combustion products, P, are delineated on the diagram of states portrayed by Fig. 1.

The state coordinates of F and A are prescribed by their initial chemical composition. Coordinates of the air/fuel mixture in the system, S, or of the reactants, R, $z_M = w_M, u_M$, where $M = R, S$, are calculated for their appropriate mixture ratios according to the mixing rule

$$z_M = \frac{z_A + \sigma_M z_F}{1 + \sigma_M} \quad (7)$$

where $\sigma_M \equiv (Y_A / Y_F)_M$.

The coordinates of products, P, are determined, thereupon, by the condition of thermodynamic equilibrium attained from any state point of M, corresponding, in accordance with the phase rule, to two specified parameters of state, such as pT, hp, or uv.

Salient features of the progress of an exothermic process, taking place in the course of its dynamic stage, are exhibited by the diagram of conversion, Fig. 2, in terms of the mass fractions of components for the case of a fuel-lean charge. The degree of conversion executed by the exothermic process is expressed then in terms of a progress parameter

$$x_F(t) \equiv \frac{y_P(t)}{Y_R} \quad (8)$$

where $Y_R = (1 + \sigma_R)Y_F$. Then, as evident from Fig. 2,

$$y_F = Y_F - Y_F x_F \quad (9)$$

while

$$y_A = Y_A - \sigma_M Y_F x_F \quad (10)$$

The parameters of state identify a vector of thermodynamic properties, expressed in terms of the common variable $z_K = w_K, u_K$; the coordinates of the diagram of conversion specify a concomitant vector of components, y_K , where $K = A, F, R, P, S$. The coordinates of the system are given then by a scalar product of these vectors, so that

$$z_S = z_A y_A + z_F y_F + z_P y_P \quad (11)$$

whence, in view of (8)-(10),

$$z_S = z_A Y_A + z_F Y_F - (z_A \sigma_R Y_F + z_F Y_F - z_P Y_R) x_F \quad (12)$$

or, in terms of the vector of initial composition (associated with variable thermodynamic parameters)

$$z_I \equiv z_A Y_A + z_F Y_F \quad (13)$$

and, with y_R denoting the variable mass fraction of reactants,

$$z_R y_R \equiv (z_F + \sigma_R z_A) Y_F x_F \quad (14)$$

the state coordinates of the system are

$$z_S = z_I + (z_P - z_R) Y_R x_F \quad (15)$$

An inverse problem for a closed combustion system involves the determination of the progress of the dynamic stage of combustion expressed by the profiles of all the thermodynamic parameters, as well as the kinetics of fuel consumption, from the measured pressure profile. One should keep in mind that, in the analysis, all the thermodynamic parameters are expressed with respect to a unit mass of the chemical system.

Under such circumstances, for $z = w$, (15) expresses the **balance of volume**, so that

$$w_P = w_M + \frac{w_S - w_I}{Y_M x_F} \quad (16)$$

For $z = u$, (15) provides also an expression for the change in internal energy of the system

$$u_S = u_I - (u_M - u_P) Y_M x_F \quad (17)$$

Hence, the **energy balance** means simply that in an isochoric and adiabatic case under consideration, $u_S = u_{Si}$, so that

$$(\mathbf{u}_M - \mathbf{u}_P)Y_M \mathbf{x}_F - (\mathbf{u}_I - \mathbf{u}_{Si}) = 0 \quad (18)$$

If the loci of states on the state diagram can be linearised, this expression can be simplified by the introduction of their slopes, C_K ($K = M, P$) and the ordinates of their tangents at $w = 0$, u_{K0} . The jump, expressed by $q_M = u_{M0} - u_{P0}$, is thus, *de facto*, a geometric parameter, expressing what is popularly referred to as "heat release" - a well-established terminology that often leads to confusion. Perhaps a better term would be "exothermic energy," but, irrespectively how it is called, its basic nature is that of a measure of a shift on the diagram of states, in either $\mathbf{u}-\mathbf{w}$ or $\mathbf{h}-\mathbf{w}$ coordinates.

Thus

$$\mathbf{u}_M = C_M \mathbf{w}_M \quad \text{while} \quad \mathbf{u}_P = C_P \mathbf{w}_P - q_M \quad (19)$$

so that

$$\mathbf{u}_M - \mathbf{u}_P = C_M \mathbf{w}_M - C_P \mathbf{w}_P + q_M \quad (20)$$

while

$$\mathbf{u}_U - \mathbf{u}_{Si} = C_M (\mathbf{w}_U - \mathbf{w}_{Si}) \quad (21)$$

whence the energy balance of (18) becomes

$$(C_M \mathbf{w}_M - C_P \mathbf{w}_P + q_M)Y_M \mathbf{x}_F - C_M (\mathbf{w}_I - \mathbf{w}_{Si}) = 0 \quad (22)$$

Then, upon eliminating of \mathbf{w}_P by the virtue of (16),

$$[q_M - (C_P - C_M) \mathbf{w}_M]Y_M \mathbf{x}_F = C_P (\mathbf{w}_S - \mathbf{w}_U) - C_M (\mathbf{w}_I - \mathbf{w}_{Si}) \quad (23)$$

whence, taking into account the effectiveness of the dynamic stage, η_F ,

$$\mathbf{x}_F = \frac{1}{\eta_F Y_M} \frac{C_P (\mathbf{w}_S - \mathbf{w}_U) + (C_P - C_M) (\mathbf{w}_I - \mathbf{w}_{Si})}{q_M - (C_P - C_M) \mathbf{w}_M} \quad (24)$$

or, in a form normalized with respect to w_{Si} , while the process of compression is expressed by a polytrope, according to which $\mathbf{w}_U / w_{Si} = \mathbf{w}_M / w_{Si} = \mathbf{P}^\alpha$, where, with n_M denoting the polytropic index, $\alpha \equiv 1 - n_M^{-1}$, in terms of $\mathbf{P} \equiv p / p_i$, $Q_M \equiv q_M / w_{Si}$,

$$\mathbf{x}_F = \frac{1}{\eta_F Y_M} \frac{C_P (\mathbf{P} - 1) + (C_P - C_M) (\mathbf{P}^\alpha - 1)}{Q_M - (C_P - C_M) \mathbf{P}^\alpha} \quad (25)$$

Solution*

The inverse problem we addressed was to deduce data specifying the kinetics of fuel consumption, as well as the evolution of thermodynamic state parameters, from mass spectroscopic measurements of the composition of the detonation products and the transducer records of pressure profiles.

The analytical gas mass spectroscopy measurements yielded the volumetric fractions, X_{oi} , in terms of: 0.72 CO₂, 0.84 CO, 0.05 CH₄, 0.26 H₂, 0.02 O₂, and 98.11 N₂. On this basis, (3)-(6) yielded $\alpha = 1.879$, as well as $v_6 = 178.5$, $v_7 = 4.12$ and $v_8 = 1.86$, so that, according to (2),



for which $\sigma_R = 3.17$. The composition of the fuel for the ensuing process of combustion, thus determined, was found to be in a satisfactory agreement with the results of the computations made by the use of CHEETAH³. The latter were carried out for isentropic expansion of detonation products from the Chapman-Jouguet state to initial conditions of the dynamic stage of combustion. The state coordinates of F and A, as well as of P, were evaluated then by the use of STANJAN⁴, while those of S and R were deduced from the data for F and A by means of (7).

*As appropriate for an abstract, provided here are only highlights of the results we obtained. Their complete set and numerical background, as well as answers to any questions an interested reader may pose, are readily obtainable by demand addressed to ako@me.berkeley.edu

³ Fried, L.E., *Cheetah 1.22*, LLNL Publication, 185 pp., 1995

⁴ Reynolds, W.C., *STANJAN*, Department of Mechanical Engineering, Stanford University, 48 pp., 1986

The pressure records were obtained from four test runs in air and four in nitrogen. The latter provided the base line for the pressure profile of the dynamic stage of combustion in the shock compressed air recorded by the former. In both cases, they were obscured initially by high amplitude fluctuations due to the oscillating shock fronts, produced by the blast wave generated by the explosion of the TNT charge. Upon this relatively short period of this noise, the rest of the data were time-averaged. The results are presented in Fig.3, where $t = 0$ marks their delayed start. As evident there, the initial point was then determined by the intersection of the pressure profile and its base. Presented there also is a hypothetical pressure profile, which would have been obtained in the absence of dilution by the large excess of air contained in the test vessel.

The experimental test was carried out with a TNT/air mass ratio of $\sigma = 18.5$. The initial pressure for combustion following the explosion was $p_i = 1.74$ atm, at a temperature of $T_i = 444$ K, while the maximum pressure was recorded at a level of $p_e = 3.75$ atm, as displayed in Fig. 3. The corresponding state diagram of the system and its components is presented by Fig. 4. To comply with the measured pressure data, it was found that $\sigma_s = 22.4$, $q_s = 0.48$ kJ/g, $C_s = 2.71$ and $C_{ps} = 3.01$. The discrepancy between the mass ratio deduced from recorded pressures and that of the initial charge is interpreted as a measure of the effectiveness of the dynamic stage of combustion. Its value of $\sim 80\%$ is due, most probably, to the depletion of carbon by its deposition on the walls - an effect that is quite apparent upon opening the explosion vessel after the test. Delineated also on Fig. 4 are the states attainable by a stoichiometric reaction corresponding to $\sigma_R = 3.17$, for which $p_f = 9.59$ atm (displayed in Fig. 3), $q_R = 3.33$, $C_R = 2.99$ and $C_p = 5.42$.

On this basis, the mass fraction of consumed fuel was evaluated according to (25), whence the effectiveness of the dynamic stage of combustion was found to be $\eta_F = 0.926$. The profile of fuel consumption was then expressed in terms of the life function - a kinematic expression for the kinetic process of combustion, introduced in our previous publications cited in the footnote on p.1, i.e.

$$x = \frac{e^{\zeta} - 1}{e^{\zeta_f} - 1} \quad \text{where} \quad \zeta = \frac{\alpha}{\chi + 1} [1 - (1 - \tau)^{\chi + 1}] \quad \text{while} \quad \tau \equiv \frac{t - t_i}{t_f - t_i}, \quad (26)$$

with $\alpha = \chi = 1.5$. The resultant mass fraction and rate of fuel consumption are displayed by Fig. 5, while the concomitant profiles of the temperatures and densities are depicted on Fig. 6, completing thus our report on the solution of the inverse problem posed at the outset.

Nomenclature

C_K slope of a locus of states
 p pressure
 $q_M \equiv u_{M0} - u_{P0}$
 t time
 T temperature
 u_K internal energy
 v_K specific volume
 $w_K \equiv p_K v_K$
 x progress parameter
 X_i volumetric fraction
 y_K variable mass fraction
 Y_K fixed mass fraction
 $z_K = w_K, u_K$
 α stoichiometric variable
 life function parameter
 χ life function parameter
 η_F effectiveness
 v stoichiometric coefficient

ρ density
 σ_M air/fuel mass ratio
 ζ life function exponent
Designations
 A air
 F fuel
 f final
 i initial
 K \equiv A, F, M P, R, S
 M \equiv R, S
 Mo coordinate of M at $w = 0$
 P products
 Po coordinate of P at $w = 0$
 P_R equilibrium products of R
 P_S equilibrium products of S
 R reactants
 S system
 U unconverted component

